

Citric acid  
77-92-9 | DTXSID3020332

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 318 °C

Global applicability domain: Outside

Local applicability domain index: 1.22e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Heptanedioic acid</div> <div>Measured: 342</div> <div>Predicted: 332</div>	<div>Image not found</div> <div>Hexanedioic acid</div> <div>Measured: 338</div> <div>Predicted: 330</div>	<div>Image not found</div> <div>Octanedioic acid</div> <div>Measured: 346</div> <div>Predicted: 332</div>
<div>Image not found</div> <div>Pentanedioic acid</div> <div>Measured: 303</div> <div>Predicted: 310</div>	<div>Image not found</div> <div>3-Ethyl-3-methylglutaric acid</div> <div>Measured: 261</div> <div>Predicted: 286</div>	